ELAIDIC ACID

Mol. wt. 282.5 (c<sub>18</sub>H<sub>34</sub>O<sub>2</sub>)

Submitted by Daniel Swern and John T. Scanlan, Eastern Regional Research Laboratory, Philadelphia. Checked by Charles C. Sweeley and H. E. Carter, University of Illinois, Urbana.

I. Principle

(Se)

$$cH_{3}(cH_{2})_{7}cH=cH(cH_{2})_{7}cO_{2}H(cis) \xrightarrow{CH_{3}(cH_{2})_{7}cH=cH(cH_{2})_{7}cO_{2}H(trans)}$$

Oleic acid is isomerized to the trans elaidic acid by a variety of reagents, of which selenium is the most convenient. The conversion is an equilibrium reaction, and the equilibrium mixture contains about 67% of elaidic acid.

## II. Starting Material

Oleic acid of 94-97% purity may be prepared as described in Biochemical Preparations, 2, 100 (1952). If this material is not available, red oil (commercial product containing 60-75% oleic acid) may be employed. However, it is necessary to crystallize the elaidinization product two to three times from acetone at -20° and once or twice at 0° to -5° to obtain a pure product, and the yield is only 30% when red oil is the starting material.

An excellent alternative starting material is the filtrate fraction obtained when the bulk of the saturated fatty acids of beef tallow fatty acids have been removed by precipitation from acetone at  $-20^{\circ}$  (6 ml. of acetone per gram of solute). The elaidinization product is crystallized twice from acetone at  $-20^{\circ}$  and once at  $0^{\circ}$  to  $-5^{\circ}$ .

<sup>1.</sup> For references see A. W. Ralston, Fatty Acids and Their Derivatives, pp. 110-111, John Wiley & Sons, 1948.

<sup>2.</sup> H. N. Griffiths and T. P. Hilditch, J. Chem. Soc., 1932, 2315.
3. D. Swern, H. B. Knight, J. T. Scanlan, and W. C. Ault, Oil & Soap, 22, 302 (1945).

## III. Procedure

In a 500-ml, three-necked flask equipped with an air condenser, a thermometer, and a gas inlet tube which reaches to the bottom of the flask, 4200 gm. of oleic acid (purity 94-97%) and 0.6 gm. of powdered selenium are heated for 1 hour at 220-225° in an atmosphere of carbon dioxide or nitrogen. This operation should be carried out in a hood. The reaction mixture, after cooling to about 50°, is dissolved in 1000 ml of acetone (5 ml. per gm. of solute), and 4 gm. of activated carbon are added. The solution is allowed to stand for about 1 hour with occasional shaking and is then filtered. The filtrate is cooled to 0° to -5°, and the crystalline precipitate is filtered by suction, washed with about 100 ml. of acetone at 0°, and air-dried, giving 83-85 gm. of almost pure elaidic acid melting at 43-45° and giving an iodine number of about 88. The yield is 62-64%, based on the assumption that only 67% of the cleic acid is elaidinized. Recrystallization of this product from acetone gives pure elaidic acid melting at 44-45° (yield, 62-64 gm.).

## IV. Properties and Purity of Product

Pure elaidic acid melts at 44.5° and distils without decomposition under reduced pressure (b.p. 225°/10 mm., 252°/30 mm.). The iodine number is 89.9. Elaidic acid in mixtures of cis and saturated fatty acids is best determined by spectrophotometric analysis.

## V. Methods of Preparation

Oleic acid may be elaidinized by selenium and by oxides of nitrogen and sulfu.

<sup>4.</sup> Mechanical agitation is not required if the inert gas enters near the bottom of the reaction flask.

<sup>5.</sup> The selenium (m.p. 217°) melts during the heating.

<sup>6.</sup> D. Swern, H. B. Knight, O. D. Shreve, and M. R. Heether, J. Am. Oil Chemists: Soc., 27, 17 (1950); O. D. Shreve, M. R. Heether, H. B. Knight, and D. Swern, Anal Chem., 22, 1261 (1950).

<sup>7.</sup> S. H. Bertram, Chem. Weekblad, 33, 3 (1936).

<sup>8.</sup> K Lutenberg, Fettchem. Umschau, 42, 89 (1935).

<sup>9.</sup> G. Rankov. Ber. deut. chem. Ges., 62, 2712 (1929); 64, 619 (1931).